On the replica method for glassy systems

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Abstract

In this talk we review our theoretical understanding of spin glasses paying a particular attention to the basic physical ideas. We introduce the replica method and we describe its probabilistic consequences (we stress the recently discovered importance of stochastic stability). We show that the replica method is not restricted to systems with quenched disorder. We present the consequences on the dynamics of the system when it slows approaches equilibrium are presented: they are confirmed by large scale simulations, while we are still awaiting for a direct experimental verification.

1 INTRODUCTION

It is a sad occasion to speak at this meeting. Giovannino was a student of mine during the first year I was giving a course at the university (in 1979). It was a particular occasion for me (my first teaching as a professor) and I have a vivid memory of him during that course, of his positive attitude toward life, of his smiling. Later Giovannino went on his road which was different but nearly parallel to mine. We have written a few papers together [1] and I remember with great pleasure this collaboration. Just a few days before his unexpected death, we spent more than an hour discussing his recent work on spin glasses [2] and the possibility of extending it to the case of spontaneous breaking of the replica symmetry.

In this talk I will present a short introduction to the replica method for glassy system, concentrating on the physical ideas; I have tried to organize this in such a way that i believe it should have pleased Giovannino, if he were present.

In section II we introduce the replica method and we describe its probabilistic consequences. In section III we define a recently discovered property (stochastic stability) and we show its great relevance in understanding the properties of disordered systems. In section IV we present some of the considerations that imply that the replica method is not restricted to systems with quenched disorder. In section V we spell out the consequences of the replica approach on the dynamics of the system when it slows approaches equilibrium are presented and we show that they are confirmed by large scale simulations. Finally, in section VI, we present our conclusions.

2 THE REPLICA METHOD

The basic idea of the replica method is quite simple. We consider a function $F(n)$ defined on the integers; using some property of this function, we extend it to real numbers.

As far I can tell the first use of the replica method goes back to Nicola d'Oresme, bishop of Lisieux (1330-1378). He made the following observation. It well known that

$$(a^m)^n = a^{mn} \tag{1}$$

for integer n. If we suppose that a^m make sense also for rational non-integer m, the previous property allow its computation. For example using

$$(a^{1/2})^2 = a, \tag{2}$$

we find that

$$a^{1/2} = \sqrt{a}. \tag{3}$$

The same procedure can be used in the study of disordered systems [3, 4]. In this case we have an Hamiltonian $H_J(\sigma)$ in which the J are some control variables (which are distributed according to the probability $P(J)$) and the $\sigma(i)$ ($i = 1, N$) are the dynamical variables. We define

$$Z_J = \sum_{\{\sigma\}} \exp(-\beta H_J(\sigma)) \equiv \exp(-\beta N F_J). \tag{4}$$

Our goal is to compute

$$\overline{F} \equiv \int dP(J) F_J. \tag{5}$$

(the bar denotes the average of the control variables J).

At this end we introduce for real n the function $F(n)$ defined as

$$F(n) = -\frac{\ln\left(\overline{Z_J^n}\right)}{n\beta N} \ . \tag{6}$$

The value of $F(0)$ can be defined by continuity in n and we find that

$$F(0) = \overline{F}. \tag{7}$$

On the other hand for integer n we can introduce n replicas of the same system (which will be labeled by $a = 1, n$) and can write

$$\overline{Z_J^n} = \overline{\prod_{a=1,n} \left(\sum_{\{\sigma^a\}}\right) \exp(-\beta \sum_{a=1,n} H_J(\sigma_a))} = \prod_{a=1,n} \left(\sum_{\{\sigma^a\}}\right) \exp(-\beta H_{eff}(\sigma)) \tag{8}$$

where $H_{eff}(\sigma)$ depends on the σ-variables in all the n replicas. For example if

$$H = \sum_{i,k=1,N} J_{i,k} \sigma_i \sigma_k, \tag{9}$$

we have that

$$H_{eff}(\sigma) = \sum_{a,b=1,n} \sum_{i,k=1,N} \sigma_i^a \sigma_k^a \sigma^b i_i \sigma_k^b. \tag{10}$$

There are many systems whose dynamics becomes very slow at low temperature. Some of these systems clearly display a thermodynamic transition (as can be seen by many effects, e.g. discontinuities in the specific heat, sharp peaks in the susceptibilities or divergences in non linear susceptibilities). However by lowering the temperature we do not produce an ordered state like a crystal.

The aim of the replica theory is to describe this transition and the system below the transition.

Let us first recall the description of these glassy systems at equilibrium in the low energy phase according to the predictions of the replica theory. We consider a given system and we denote by $\mathcal{C}$ a generic configuration of the system. For simplicity we will assume that there are no symmetry in the Hamiltonian (in presence of symmetries the arguments must be slightly modified).

It is useful to introduce an overlap $q(\mathcal{C}, \mathcal{C}')$. There are many ways in which an overlap can be defined; for example in spin system we could define

$$q = \frac{\sum_{i=1,N} \sigma_i \tau_i}{N}, \tag{11}$$

N being the total number of spins or particles and σ and τ are the spins of the two configurations.

In a liquid a possible definition of the overlap is given by

$$q = \frac{\sum_{i=1,N} \sum_{k=1,N} f(x(i) - y(k))}{N}, \tag{12}$$

where $f(x)$ is a function which decays in a fast way at large distances and is substantially different from zero only at distances smaller that the interatomic distance (x and y are the coordinates of the N particles of the two configurations of the system).

In the high temperature phase for very large values of N the probability distribution of the overlap ($P_N(q)$) is given by

$$P_N(q) \approx \delta(q - q^*). \tag{13}$$

The value of q^* can be often simply computed. For example for spin systems in zero magnetic field we have $q^* = 0$. In a liquid $q^* = \rho \int d^3x f(x)$.

In the low temperature phase $P_N(q)$ depends on N (and on the quenched disorder, if it is present). When we average over N we find a function $P(q)$ which is not a simple delta function. In all known cases [3, 4, 5] one finds that

$$P(q) = a_m \delta(q - q_m) + a_M \delta(q - q_M) + p(q), \tag{14}$$

where the function $p(q)$ does not contains delta function and its support is in the interval $[q_m, q_M]$.

The non triviality of the function $P(q)$ (i.e. the fact that $P(q)$ is not a single delta function and consequently q is an intensive fluctuating quantity) is related to the existence of many different equilibrium states. Moreover the function $P_N(q)$ changes with N and its statistical properties (i.e the probability of getting a given function $P_N(q)$) can be analytically computed [3].

In this equilibrium description a crucial role is given by the function $x(q)$ defined as

$$x(q) = \int_{q_m}^{q} P(q')dq' \ . \tag{15}$$

In the simplest case the function $P(q)$ is equal to zero. i.e the function $P(q)$ has only two delta functions without the smooth part. In this case, which correspond to one step replica symmetry breaking, there are many equilibrium states, labeled by α, and the overlaps among two generic configurations of the same state and of two different states are respectively equal to q_M and q_m. The probability $\mathcal{P}(f)$ of finding a state with total free energy f is proportional to

$$\mathcal{P}(f) \propto \exp\left(m\beta(f - f_R)\right), \tag{16}$$

where f_R is a reference free energy and m is the value of $x(q)$ in the interval $[q_m, q_M]$.

In the more complicated situation where the function $p(q)$ is non zero, couples of different states may have different values of the overlaps. The conjoint probability distribution of the states and of the overlaps can be described by formulae similar to eq. (16), but more complex [3].

3 STOCHASTIC STABILITY

Stochastic stability is a property which is valid in the mean field approximation; it is however possible to conjecture that is valid in general also for short range models. It has been introduced quite recently [6, 7, 8, 9] and strong progresses have been done on the study of its consequences.

In order to decide if a system with Hamiltonian H is stochastically stable, we have to consider the free energy of an auxiliary system having the following Hamiltonian:

$$H + \epsilon^{1/2} H_R. \tag{17}$$

If the average (with respect to H_R) free energy is a differentiable function of ϵ (and the limit volume going to infinity commutes with the derivative with respect to ϵ), for a generic choice of the random perturbation H_R inside a given class and ϵ near to zero, the system is stochastically stable.

The definition of stochastic stability may depend on the class of random perturbations we consider. Quite often it is convenient to chose as a random perturbation an infinite range Hamiltonian, e.g.

$$H_R = \sum_{i,k,l} J_{i,k,l} \sigma_i \sigma_k \sigma_l \tag{18}$$

where sum runs over all the N points of the system and the J's are random variables with variance $1/N$.

In the nutshell stochastic stability tell us that the Hamiltonian H does not has any special features and that it properties are quite similar to those of similar random systems.

Although it seems quite natural, stochastic stability has quite deep consequences. For example we could consider a system in which there are many equilibrium states, labeled by α, and the overlaps among two generic configurations of the same state and of two different states are respectively q_M and q_m, the free energies of the different states are uncorrelated... The situation would be quite similar to the one described by one step replica symmetry breaking. However we may not specify the form of the probability distribution of the free energies which is characterized by a function $\mathcal{P}(f)$ which a priori may have an arbitrary shape.

It is a simple computation to verify that stochastic stability implies that the probability distribution of the free energies ($\mathcal{P}(f)$) must have the form given in eq. (16) with an appropriate choice of m. The most dramatic effect of stochastic stability is to link the behaviour of the function $\mathcal{P}(f)$ in the region of large f (where a large number of states do contribute) to the low f behaviour, which controls the distribution of the states which are dominant in the partition function.

We have seen that stochastic stability strongly constraints the properties of the systems and many of the qualitative results of the replica approach can be derived as mere consequences of stochastic stability. Stochastic stability apparently does not imply ultrametricity, which seems to be an independent property [8]. This independence problem is still open as far has the only explicitly constructed probabilities distribution of the free energies of the states are ultrametric.

4 SYSTEMS WITOUT QUENCHED DISORDER

Apparently the previous discussions are restricted to systems where quenched disorder is present. The requirement of quenched disorder would limit ourselves in the applications of the replica method and one would cut all those systems, like glasses, which have a translational invariant Hamiltonian and where no quenched disorder is present.

This prejudice (on the need of quenched disorder(was so strong that it took a few years to realize that the replica method can also applied to system without quenched disorder.

There are many facts that clearly indicate the possibility of applying the replica methods to non-random systems.

- In the infinite range case there are pairs of systems with Hamiltonian respectively H_Q and H, where H_Q contains quenched disorder and no disorder is present in H, such the high temperature expansion for the two systems coincide [10, 11]. It is natural to suppose that the free energies of the two system are identical at all temperatures, so that replica symmetry breaking can be applied to both.

- It is possible to look for replica symmetry breaking in the expression for the free energy systems without disorder (e.g. soft spheres) inside a given approximation (e.g. hypernetted chain) and find out that replica symmetry breaks at low temperature [12].

- In the replica method we can introduce coupled replica potentials [13] in order to characterize the phase space of the system and these potentials can also be computed for non-random systems, obtaining the same results as for random systems [14]. This may be done analytically for soft spheres using the same approximation as before [15].

- It is now clear that the replica method may be applied any stochastic stable system. Indeed stochastic stable systems are the limit of disorder systems where the replica method can be applied without problems. Systems without quenched disorder may be stochastically stable if the free energy is computed using the Cesareo limit (i.e. averaging over N).

This new perspective allows us to use the replica method in systems quite different from the usual one, e.g. structural glasses, where no quenched disorder is present.

5 A DYNAMICAL APPROACH

Although the predictions of the previous sections are quite clear, it is not so simple to test them for many reasons:

- They are valid at thermal equilibrium, a condition that is very difficult to reach for this kind of systems, also in real experiments.

- Experimentally is extremely difficult to measure the values of the microscopic variables, i.e all the spins of the system at a given moment. These measurements can be done only in numerical simulations, where the observation time cannot be very large and only systems with less that 10^4 degrees of freedom may be carried to thermal equilibrium.

A very important progress has been done when it was theoretically discovered that during the approach to equilibrium of the system, the fluctuation dissipation theorem is no more valid and the function $X(C)$, which describes the violations of the fluctuation dissipation theorem, (in some mean field models) is equal to the function $x(q)$ which is relevant for the statics [16, 17]. This equality is very interesting because function $X(C)$ can be measured relatively easily in off-equilibrium simulations [19].

The temperature dependence of the function $X(C)$ (or equivalently $x(q)$) is interesting also because rather different systems can be classified in the same universality class according to the behaviour of this function. It has been conjectured long time ago that the equilibrium properties of glasses are in the same universality class of some simple generalized spin glass models [20].

Let us be more precise. We concentrate our attention on a quantity $A(t)$. We suppose that the system starts at time $t = 0$ from an initial condition and subsequently it remains at a fixed temperature T. If the initial configuration is at equilibrium at a temperature $T' > T$, we observe an off-equilibrium behaviour. We can define a correlation function

$$C(t, t_w) \equiv \langle A(t_w)A(t + t_w)\rangle \tag{19}$$

and the relaxation function

$$G(t, t_w) \equiv \left.\frac{\delta\langle A(t + t_w)\rangle}{\delta\epsilon(t_w)}\right|_{\epsilon=0}, \tag{20}$$

where we are considering the evolution in presence of a time dependent Hamiltonian in which we have added the term $\int dt\epsilon(t)A(t)$.

The usual equilibrium fluctuation-dissipation theorem (FDT) tells us that

$$G^{eq}(t) = -\beta\frac{dC^{eq}(t)}{dt}, \tag{21}$$

where

$$G^{eq}(t) = \lim_{t_w\to\infty} G(t, t_w), \quad C^{eq}(t) = \lim_{t_w\to\infty} C(t, t_w). \tag{22}$$

It is convenient to define the relaxation function:

$$R(t, t_w) = \int_0^t d\tau G(t - \tau, t_w + \tau), \quad R^{eq}(t) = \lim_{t_w\to\infty} R(t, t_w), \tag{23}$$

$R(t, t_w)$ is the response of the system at time $t + t_w$ to a field acting for a time t starting at t_w. The usual FDT relation becomes

$$R^{eq}(t) = \beta(C^{eq}(t) - C^{eq}(0)). \tag{24}$$

The off-equilibrium fluctuation-dissipation relation [16, 17] states that the response function and the correlation function satisfy the following relation for large t_w:

$$R(t, t_w) \approx \beta \int_{C(t,t_w)}^{C(0,t_w)} X(C)dC. \tag{25}$$

If we plot R versus βC for large t_w the data collapse on the same universal curve and the slope of that curve is $-X(C)$. The function $X(C)$ is system dependent and its form tells us interesting information.

In the case of spin glasses this relation was shown to be valid in the mean field approximation, however there are quite general arguments that under the appropriate hypothesis it is also valid in general (also in short range models). The proof is based on a dynamic version of stochastic stability: we must assume that in presence of a random perturbation (see eq. (18) the two limits ($t \to \infty$ and $\epsilon \to 0$) commute for the time dependent statistical expectation value of the appropriate quantities.

If we look more carefully to the graph of R versus βC we must distinguish two regions:

- A short time region where $X(C) = 1$ (the so called FDT region) and C belongs to the interval I (i.e. $C_1 < C < C_2$.).

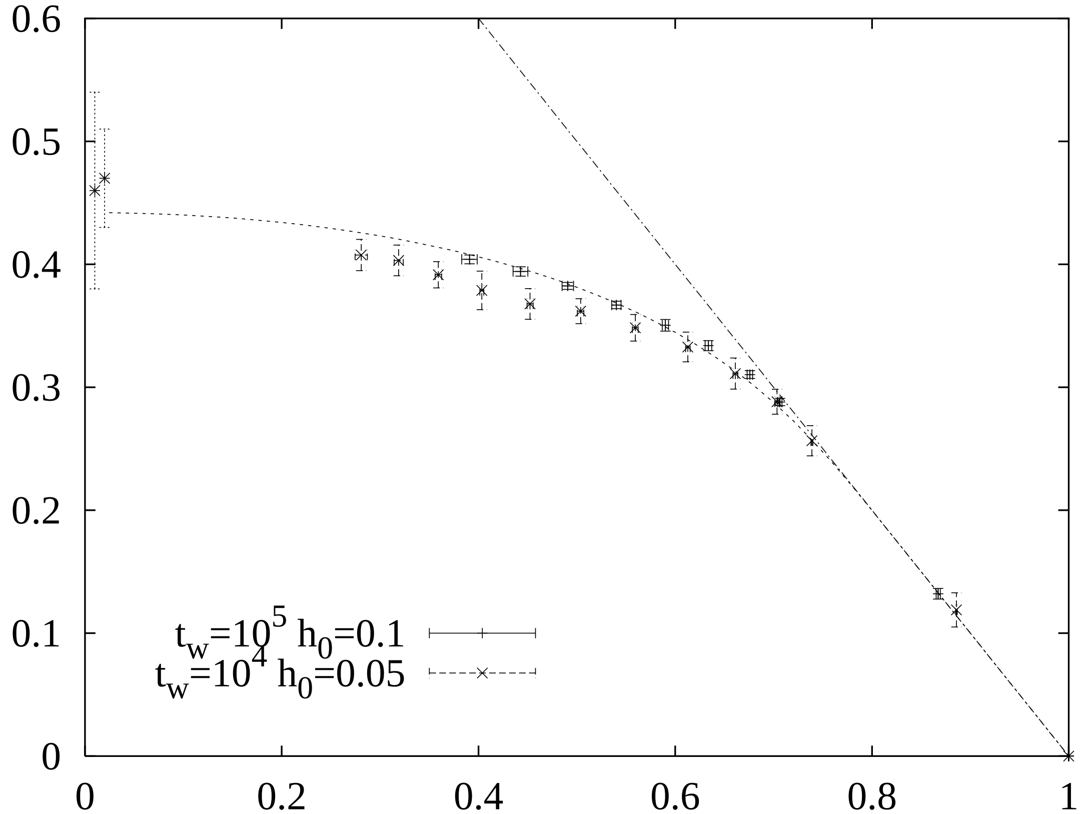

Figure 1: The relaxation R times T versus C at $T = 0.7$ for the three dimensional Ising spin glass [10]. The curve is the prediction for function $R(C)$ obtained from the equilibrium data. The straight line is the FDT prediction. We have plotted the data of the two runs: $t_w = 10^5$, and $t_w = 10^4$.

- A large time region (usually $t = O(t_w)$) where $C \notin I$ and $X(C) < 1$. In the same region the correlation function often satisfies an aging relation, i.e $C(t, t_w)$ depends only on the ration $s \equiv t/t_w$ in the region where both t and t_w are large: $C(t, t_w) \approx C^a(t/t_w)$ [18].

In the simplest non trivial case, i.e. one step replica symmetry breaking [3, 24] , the function $X(C)$ is piecewise constant, i.e.

$$X(C) = m \quad \text{for} \quad C \in I, \quad X(C) = 1 \quad \text{for} \quad C \notin I. \tag{26}$$

One step replica symmetry breaking for glasses has been conjectured in ref. [20, 21].

In all known cases in which one step replica symmetry holds, the quantity m vanishes linearly with the temperature at small temperatures. It often happens that $m = 1$ at $T = T_c$ and $m(T)$ is roughly linear in the whole temperature range.

Let us consider the case of spin glasses at zero magnetic field (in this case the replica symmetry is fully broken [5]). The natural variable to consider is a single spin ($A = \sigma_i$)). In this case the correlation $C(t, t_w)$ is equal to the overlap among two configurations at time t and t_w:

$$C(t, t_w) = \frac{\sum_{i=N} \sigma_i(t)\sigma_i(t_w)}{N}. \tag{27}$$

The response function is just the magnetization in presence of an infinitesimal magnetic field. In this case the situation is quite good because there are reliable simulations for the system at equilibrium [5].

In fig. (1) (taken from [22]) we plot the prediction for the function R versus C, obtained at equilibrium (i.e. using the equilibrium probability distribution of the overlaps, $P(q)$) by means of a simulation of a 16^3 lattice using parallel tempering [23, 5]. The simulation involves the study of 900 samples of a $L = 16$ lattice.

During the off-equilibrium simulations [22] in a first run without magnetic field the autocorrelation function has been computed. In a second second run from $t = 0$ until $t = t_w$ the magnetic field is zero and then (for $t \geq t_w$) there is an uniform magnetic field of small strength h_0. The starting configurations were always chosen at random (i.e. the system is suddenly quenched from $T = \infty$ to the simulation temperature T).

In fig. (1) there are the results of the off-equilibrium simulations [22] where $t_w = 10^5$ and $t_w = 10^4$, with a maximum time of $5 \cdot 10^6$ Monte Carlo sweeps. The lattice size in was 64^3, and $T = 0.7$ (well inside the spin glass phase, the critical temperature is close to 1.0). We plot the response function R times T (in this case R is equal to m/h_0) against $C(t, t_w)$. We have plotted also a straight line with slope -1 in order to control where the FDT is satisfied. Finally we have plotted two points, in the left of the figure, that are obtained with the infinite time extrapolation of the magnetization.

The agreement among the absolute theoretical predictions (no free parameters) coming from the statics and the dynamical numerical data is quite remarkable. These data show the correctness of the identification of the functions x of the statics and X of the dynamics.

It is quite interesting to note that numerical evaluation of the function $X(C)$ in glass forming systems (i.e. binary mixtures of soft spheres) strongly support the conjectures that glasses are systems in which the replica symmetry is broken at one step [24]. Fig. (2) shows the results for the function $R(\Delta)$ for 66 and 130 interacting particles. Here the quantity Δ plays the same role of $1 - C$ in spin glasses.The data for $R(\Delta)$ can be well fitted by two straight lines, as expected in the case of one step replica symmetry breaking

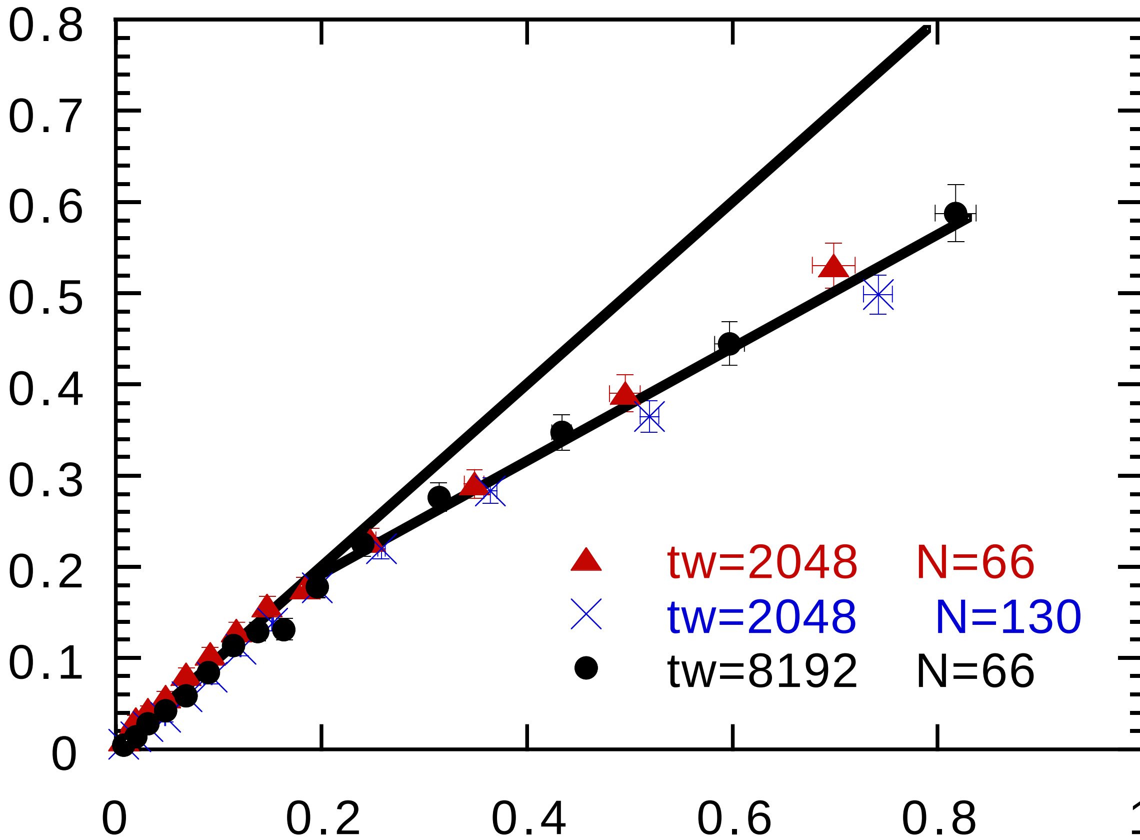

Figure 2: R versus $\beta\Delta$ at $\Gamma = 1.6$ for $t_w = 8192$ and $t_w = 2048$ at $N = 66$ and for $t_w = 2048$ at $N = 130$. The two straight lines have slope 1 and .62 respectively.

6 CONCLUSIONS

Replica theory for disordered systems provides a detailed pictures of the behaviour of glasses systems near and below the glass transition. The theoretical predictions are in very good agreement with large scale numerical simulations [5, 24]. Many of the unclear points (especially on the dynamics and on the approach to equilibrium) are now well understood.

The next step would be to test experimentally the core of the theory and to extract the function $x(q)$ from the data for the violation of the fluctuation dissipation theorem in off equilibrium dynamics. The theoretical setting is well defined, we need however carefully planned experiments in order to measure the thermal noise correlations (the response is much easier). I am confident that these experiments will be done in the next future.

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